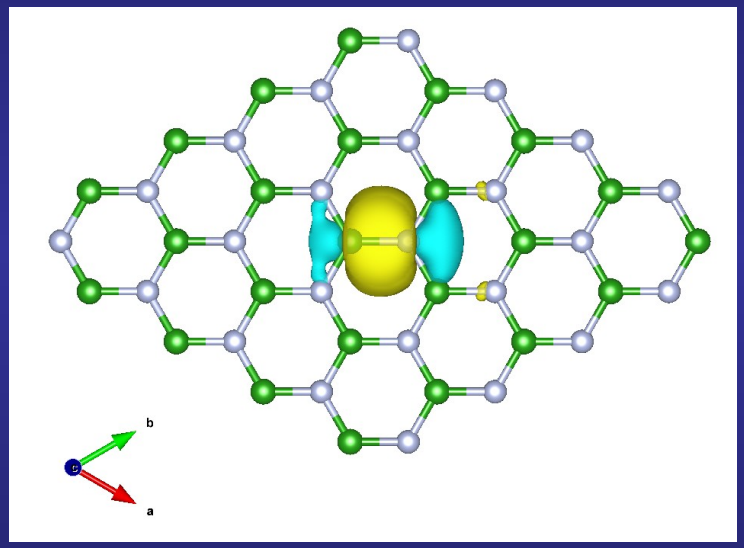
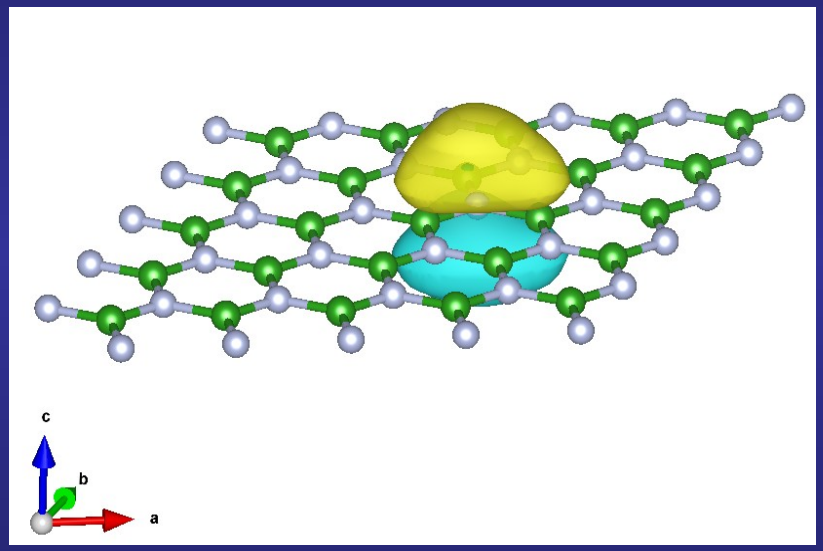
How to run WANNIER90 directly from SIESTA





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Important bibliography:

For a review on Maximally Localized Wannier functions:

REVIEWS OF MODERN PHYSICS, VOLUME 84, OCTOBER–DECEMBER 2012

Maximally localized Wannier functions: Theory and applications

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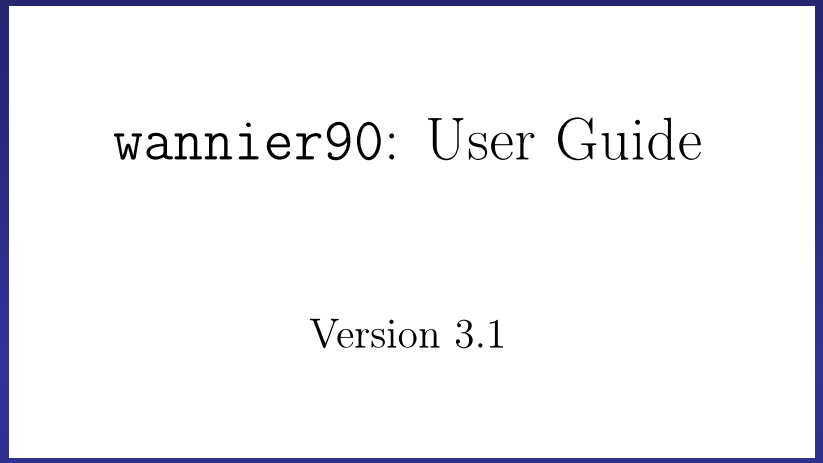
Important bibliography:

The user guide of the WANNIER90 code



Latest stable release: 5 March 2020

Released under the GNU General Public License (v2):
http://www.wannier.org

WANNIER90 code directly called from SIESTA

WANNIER90 code (version 3.1.0) has been compiled in library mode and called directly from SIESTA

That means that we can run all the functionalities of WANNIER90 directly from SIESTA

Advantages

- No need to prepare two different input files
- No need to run WANNIER90 in pre-processing mode
- We can use the basis set of SIESTA (numerical atomic orbitals) as the initial guess for the projections
- Wannierization of different manifolds can be done in the same run of SIESTA
- The unitary matrices connecting the Bloch and Wannier representations are available in SIESTA.

  New functionalities can follow (initial guesses for order-N simulations)
- Interface with other codes will be much easier:

  SCALE-UP (second-principles)

  DMFTWDFT (DMFT code by Aldo Romero's group)

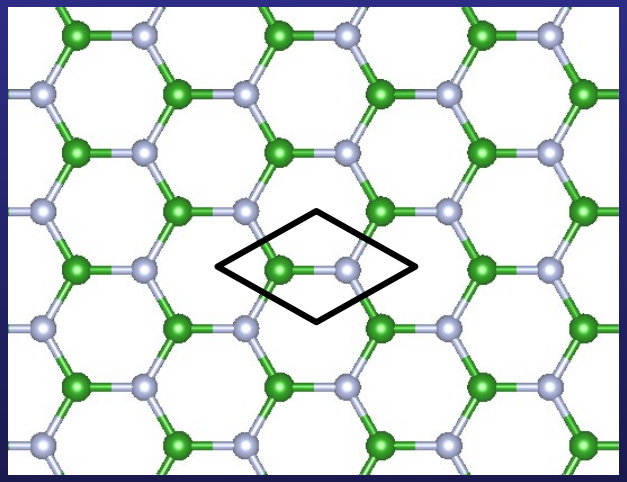
WANNIER90 code directly called from SIESTA

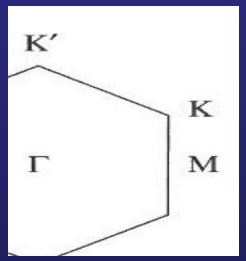
Practical examples:

h-BN

h-BN: atomic structure in SIESTA

```
# Geometry ------------------------
LatticeConstant       2.504 Ang
%block LatticeVectors
 0.86603  -0.500000  0.000000
 0.86603   0.500000  0.000000
 0.00000   0.000000  10.0
%endblock LatticeVectors
AtomicCoordinatesFormat     Fractional
%block AtomicCoordinatesAndAtomicSpecies
  0.3333333333      0.3333333333      0.0000000000  1
  0.6666666666      0.6666666666      0.0000000000  2
  0.5000000000      0.5000000000      0.0000000000  3
  0.5000000000      0.0000000000      0.0000000000  3
  0.0000000000      0.5000000000      0.0000000000  3
%endblock AtomicCoordinatesAndAtomicSpecies
```



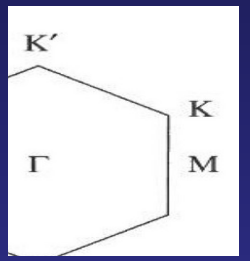


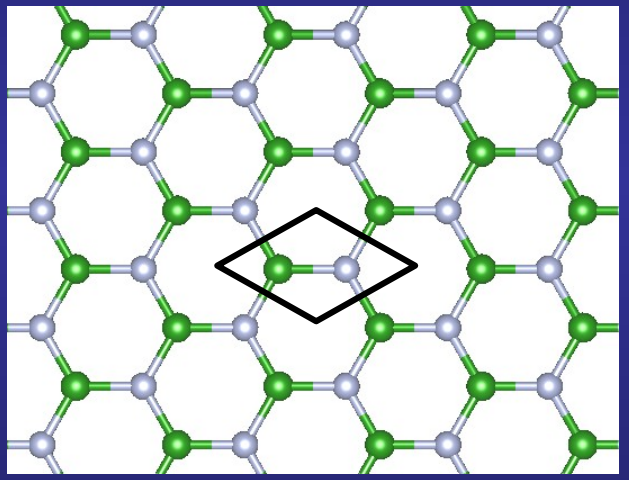
h-BN: atomic structure in SIESTA

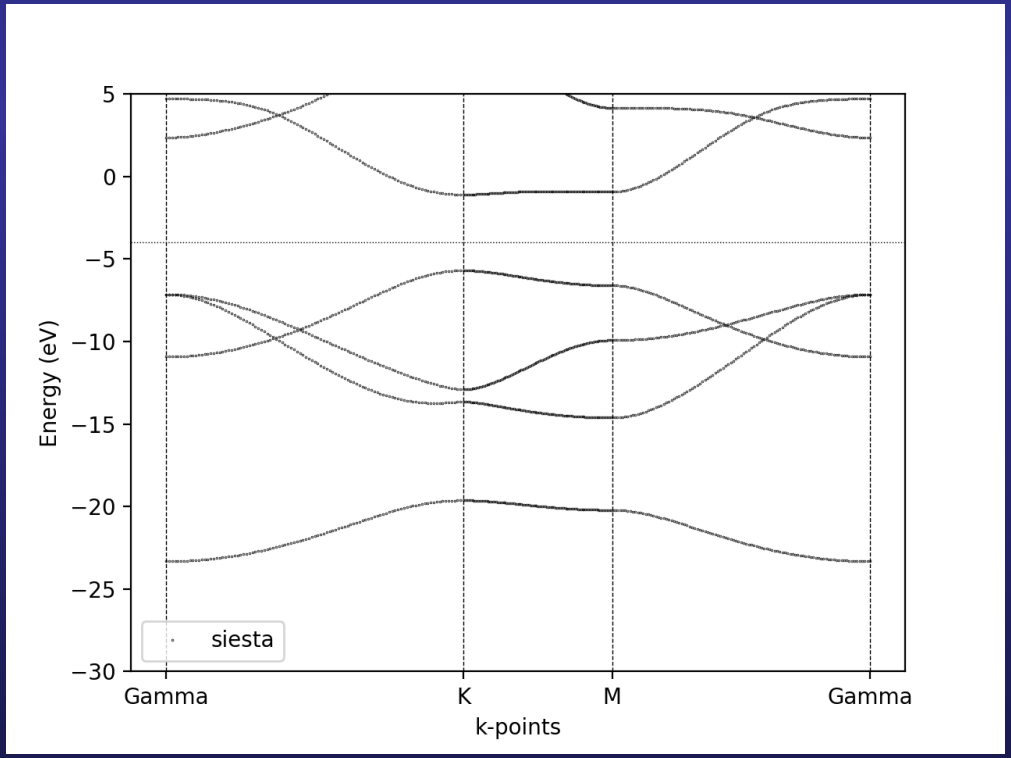
```
# Bands ----------------------------------------

BandLinesScale ReciprocalLatticeVectors

%block BandLines
1    0.000  0.000  0.000  \Gamma    # Begin at \Gamma
100  0.333  0.666  0.000  K         # 100 points from \Gamma to K
100  0.500  0.500  0.000  M         # 100 points from K to M
100  0.000  0.000  0.000 \Gamma     # 100 points from M to \Gamma
%endblock BandLines
```

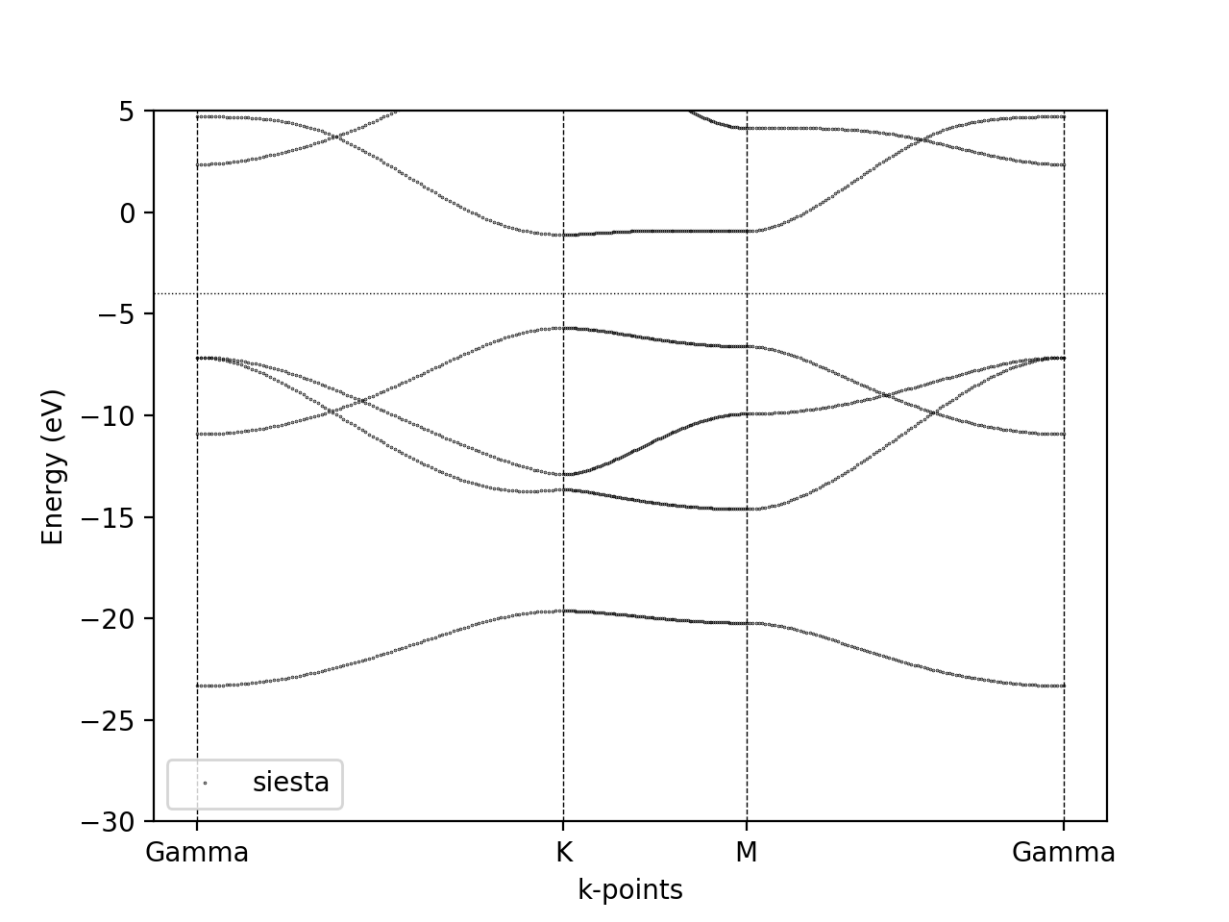






After running SIESTA and compute the fat bands, we can analyze the character of the different bands

Which atoms contribute more to the bands at a particular energy window



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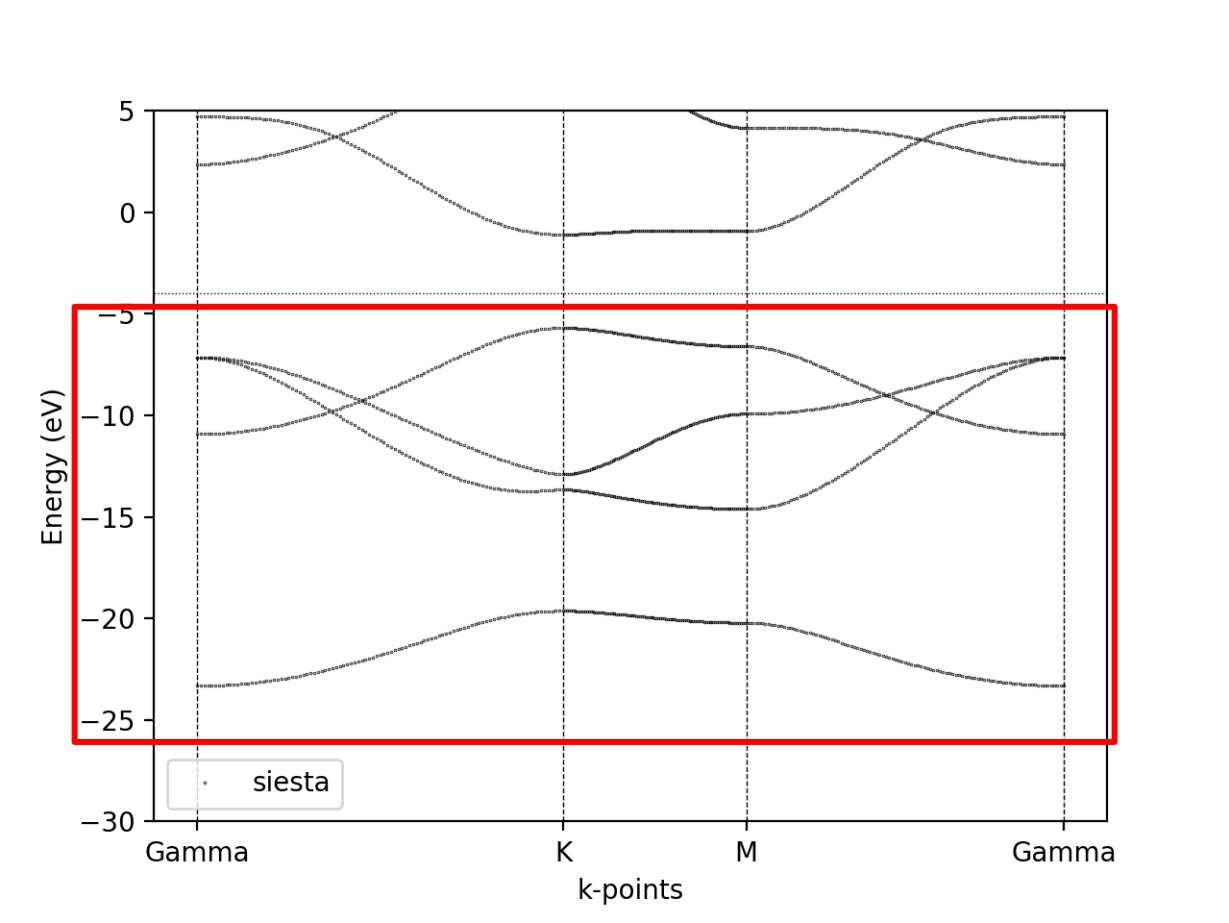


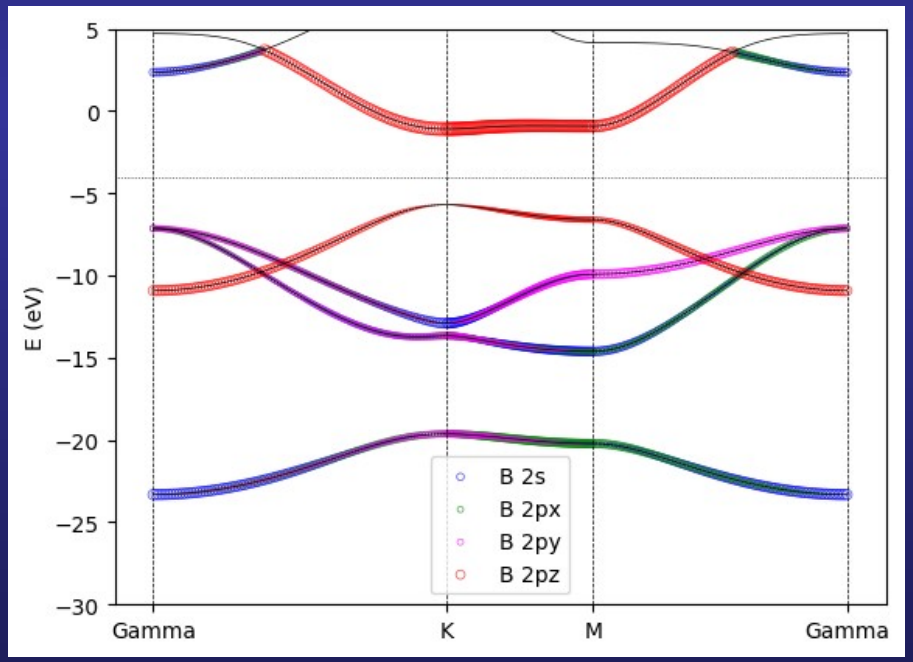
After running SIESTA and compute the fat bands, we can analyze the character of the different bands

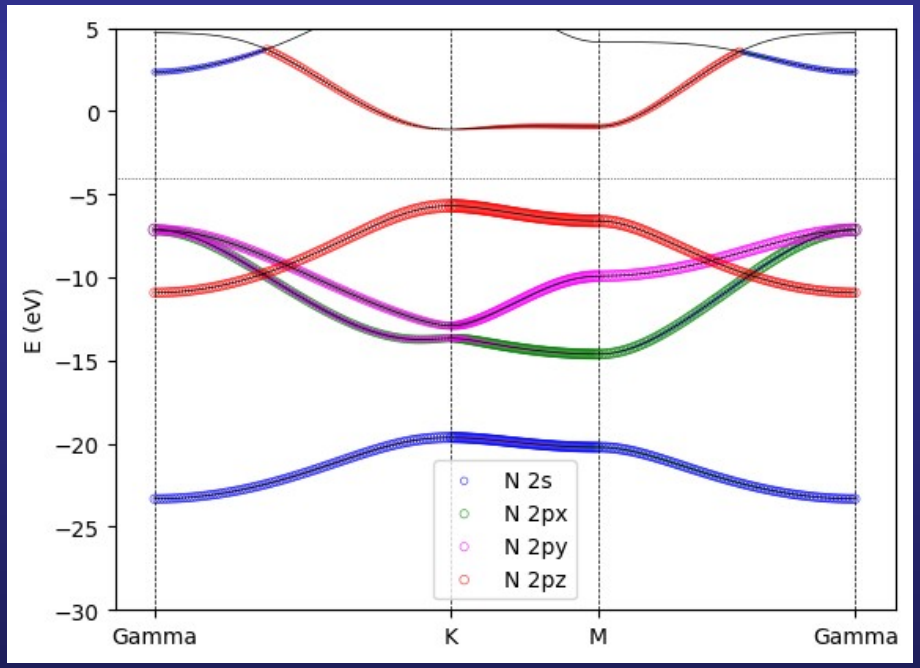
Which atoms contribute more to the bands at a particular energy window

Three bands: sp^2 character

The lower three bands have contributions from the 2s, 2px and 2py orbitals of B and N

One band : N-p_z character

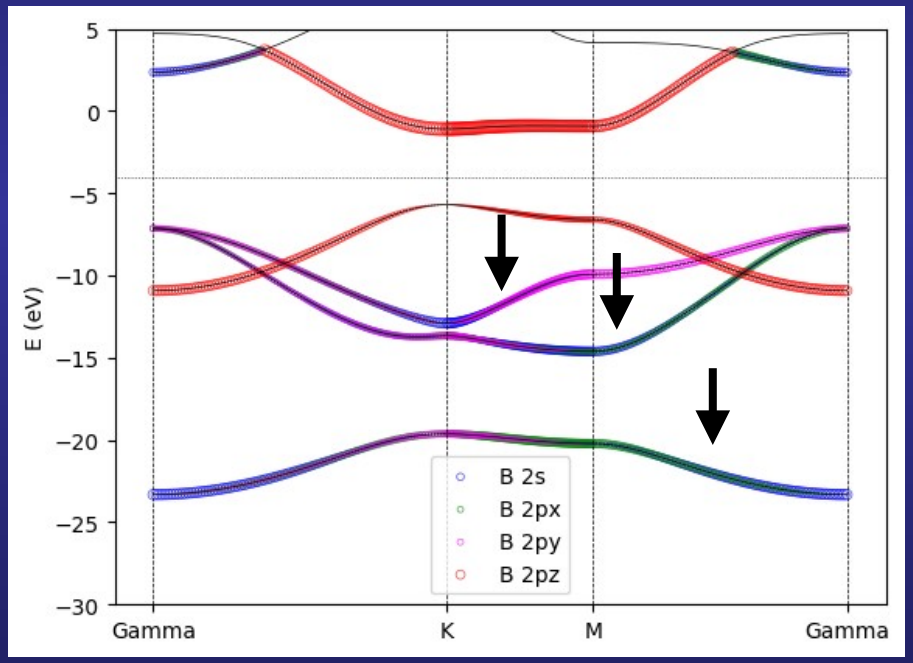


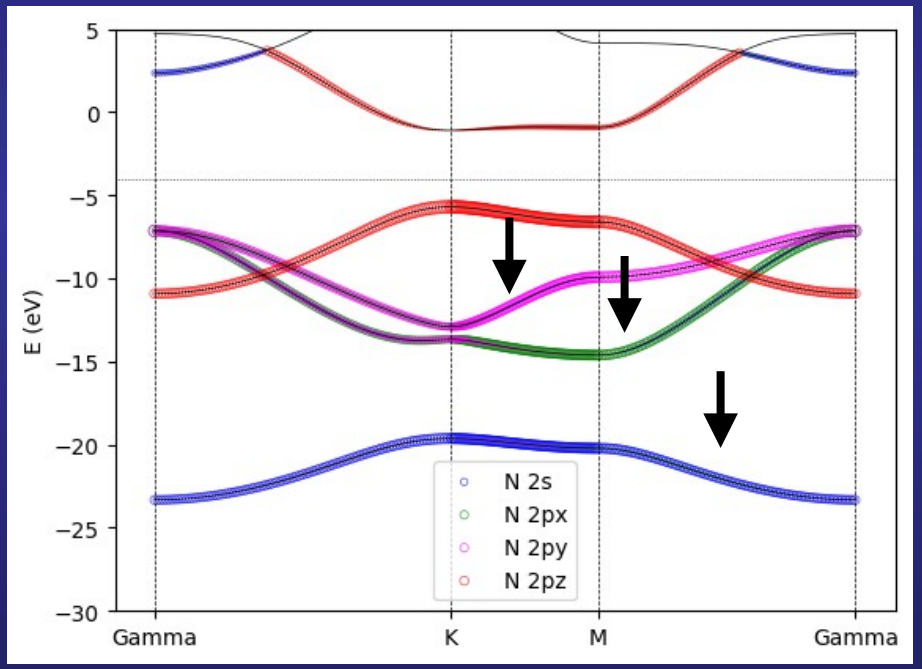


After running SIESTA and compute the fat bands, we can analyze the character of the different bands

Which atoms contribute more to the bands at a particular energy window

sp^2 orbitals of the VB are centered on the center of the B-N bonds. Then, we project onto orbitals of ghost atoms centered at these positions

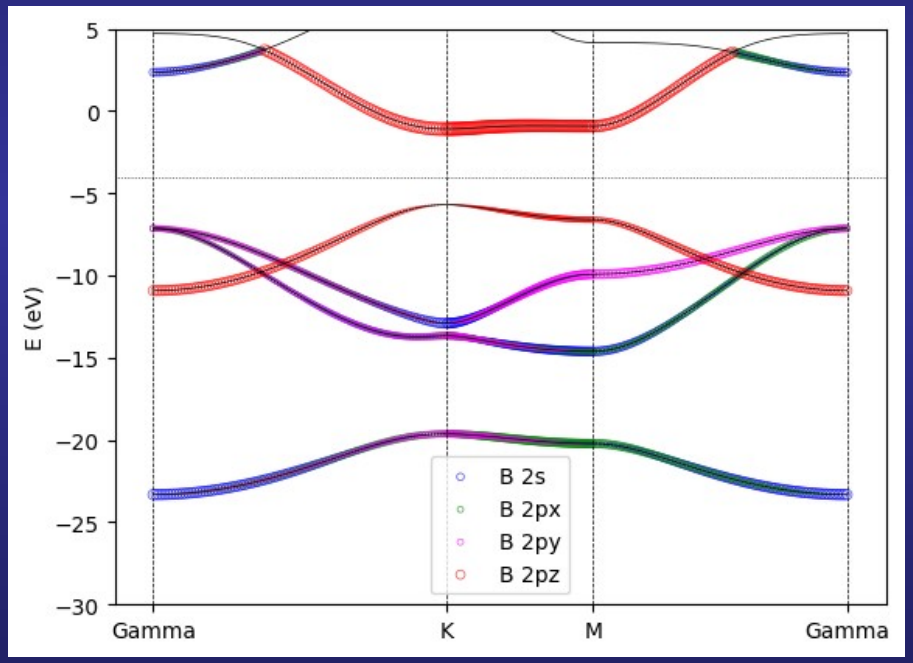


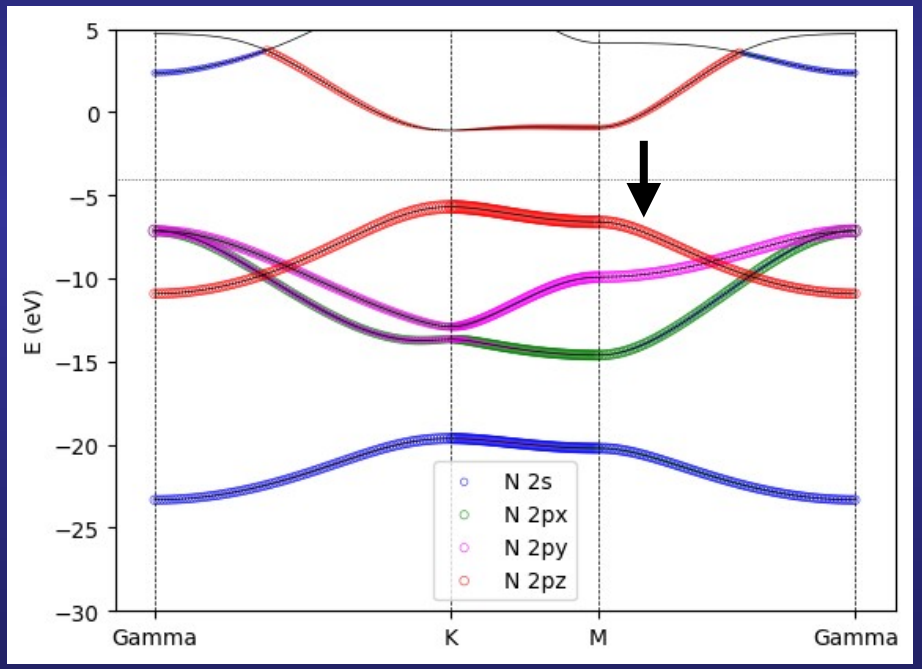


After running SIESTA and compute the fat bands, we can analyze the character of the different bands

Which atoms contribute more to the bands at a particular energy window

π-orbitals of the VB have a higher contribution from the N-p_z orbitals. Then, we project onto N-p_z orbitals.





h-BN,

including bond centered Hydrogen ghost atoms

```
SystemName          h-BN : Computation of Wannier functions
SystemLabel         h-BN

#------------------------------
# Species and atoms

NumberOfAtoms           5         # Number of atoms in the unit cell
                                  # We include here:
                                  # - The Boron atom of the motif
                                  # - The Nitrogen atom of the motif
                                  # - Three Hydrogen ghost atoms at the center
                                  #   of the bonds between first-neighbors
                                  # Only the atomic orbitals of the atoms
                                  #   will be included in the simulation,
                                  #   while the atomic nuclei will not be
                                  #   considered
NumberOfSpecies         3         # Number of different atomic species in the
                                  #   simulation.
                                  # We include here:
                                  # - B (with an atomic number of 5)
                                  # - N (with an atomic number of 7))
                                  # - pseudo-Hydrogen atom
                                  #   (with an atomic number of -1)

%block ChemicalSpeciesLabel
  1   5  B
  2   7  N
  3  -1  Ghost-H
%endblock ChemicalSpeciesLabel
```

SIESTA variables related with the wannierization

Number of manifolds to wannierize

```
%block Wannier.Manifolds
  first
%endblock
```

As many lines in the block as manifolds will be wannierized

A nickname is given to each manifold

SIESTA variables related with the wannierization

Information for every manifold

As many WannierManifolds blocks as manifolds considered for wannierization

The nickname of every manifold is appended here to the keyword WannierManifold

```
%block Wannier.manifold.first
 bands    1     4                      # Indices of the initial and final
                                       # band of the manifold
  trial-orbitals  [27, 32, 37, 20]     # Indices of the orbitals that will
                                       # be used as localized trial orbitals
                                       # See h-BN.ORB_INDX file
                                       # 27 : 1s-orbital Ghost-H atom
                                       # 32 : 1s-orbital Ghost-H atom
                                       # 37 : 1s-orbital Ghost-H atom
                                       # 20 : 2pz-orbital N atom
  spreading.nitt     0                 # Number of iterations for the minimization of \Omega
  fermi_surface_plot false             # Plot the Fermi surface (False -> NO)
  wannier_plot   3                     # Plot the Wannier function
  write_hr true                        # Write the Hamiltonian in the WF basis
  write_tb true                        # Write the Hamiltonian in the WF basis
%endblock
```

SIESTA variables related with the wannierization

```
%block Wannier.manifold.first
 bands    1     4                    # Indices of the initial and final
                                     # band of the manifold
  trial-orbitals  [27, 32, 37, 20]   # Indices of the orbitals that will
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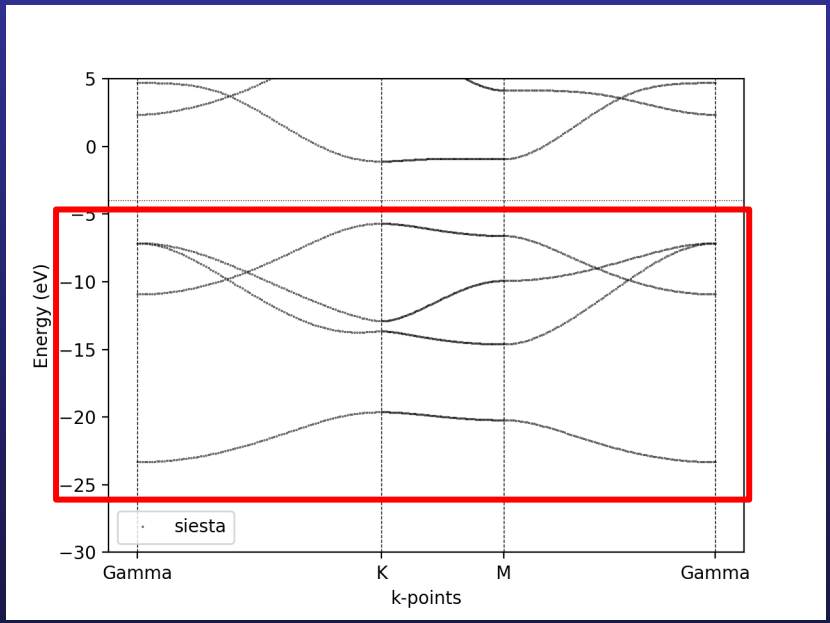
  write_hr true                      # Write the Hamiltonian in the WF basis
  write_tb true                      # Write the Hamiltonian in the WF basis
%endblock
```



SIESTA variables related with the wannierization

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%endblock
```

SIESTA variables related with the wannierization

```
  41    2009 = orbitals in unit cell and supercell. See end of file.

 io    ia is    spec iao  n  l  m  z  p          sym      rc    isc     iuo
  1     1  1       B   1  2  0  0  1  F            s   4.997  0  0  0     1
  2     1  1       B   2  2  0  0  2  F            s   3.572  0  0  0     2
  3     1  1       B   3  2  1 -1  1  F           py   5.996  0  0  0     3
  4     1  1       B   4  2  1  0  1  F           pz   5.996  0  0  0     4
  5     1  1       B   5  2  1  1  1  F           px   5.996  0  0  0     5
  6     1  1       B   6  2  1 -1  2  F           py   4.287  0  0  0     6
  7     1  1       B   7  2  1  0  2  F           pz   4.287  0  0  0     7
  8     1  1       B   8  2  1  1  2  F           px   4.287  0  0  0     8
  9     1  1       B   9  3  2 -2  1  T         Pdxy   5.996  0  0  0     9
 10     1  1       B  10  3  2 -1  1  T         Pdyz   5.996  0  0  0    10
 11     1  1       B  11  3  2  0  1  T         Pdz2   5.996  0  0  0    11
 12     1  1       B  12  3  2  1  1  T         Pdxz   5.996  0  0  0    12
 13     1  1       B  13  3  2  2  1  T      Pdx2-y2   5.996  0  0  0    13
 14     2  2       N   1  2  0  0  1  F            s   3.767  0  0  0    14
 15     2  2       N   2  2  0  0  2  F            s   2.568  0  0  0    15
 16     2  2       N   3  2  1 -1  1  F           py   4.511  0  0  0    16
 17     2  2       N   4  2  1  0  1  F           pz   4.511  0  0  0    17
 18     2  2       N   5  2  1  1  1  F           px   4.511  0  0  0    18
 19     2  2       N   6  2  1 -1  2  F           py   3.060  0  0  0    19
 20     2  2       N   7  2  1  0  2  F           pz   3.060  0  0  0    20
 21     2  2       N   8  2  1  1  2  F           px   3.060  0  0  0    21
 22     2  2       N   9  3  2 -2  1  T         Pdxy   4.511  0  0  0    22
 23     2  2       N  10  3  2 -1  1  T         Pdyz   4.511  0  0  0    23
 24     2  2       N  11  3  2  0  1  T         Pdz2   4.511  0  0  0    24
 25     2  2       N  12  3  2  1  1  T         Pdxz   4.511  0  0  0    25
 26     2  2       N  13  3  2  2  1  T      Pdx2-y2   4.511  0  0  0    26
 27     3  3  Ghost-   1  1  0  0  1  F            s   4.927  0  0  0    27
 28     3  3  Ghost-   2  1  0  0  2  F            s   3.397  0  0  0    28
 29     3  3  Ghost-   3  2  1 -1  1  T          Ppy   4.927  0  0  0    29
 30     3  3  Ghost-   4  2  1  0  1  T          Ppz   4.927  0  0  0    30
 31     3  3  Ghost-   5  2  1  1  1  T          Ppx   4.927  0  0  0    31
 32     4  3  Ghost-   1  1  0  0  1  F            s   4.927  0  0  0    32
 33     4  3  Ghost-   2  1  0  0  2  F            s   3.397  0  0  0    33
 34     4  3  Ghost-   3  2  1 -1  1  T          Ppy   4.927  0  0  0    34
 35     4  3  Ghost-   4  2  1  0  1  T          Ppz   4.927  0  0  0    35
 36     4  3  Ghost-   5  2  1  1  1  T          Ppx   4.927  0  0  0    36
 37     5  3  Ghost-   1  1  0  0  1  F            s   4.927  0  0  0    37
 38     5  3  Ghost-   2  1  0  0  2  F            s   3.397  0  0  0    38
 39     5  3  Ghost-   3  2  1 -1  1  T          Ppy   4.927  0  0  0    39
 40     5  3  Ghost-   4  2  1  0  1  T          Ppz   4.927  0  0  0    40
 41     5  3  Ghost-   5  2  1  1  1  T          Ppx   4.927  0  0  0    41
```

A good initial guess to project the bands of the three lower bands are s orbitals centered on the B-N bonds

Take a look to the SystemLabel.ORB_INDX file

s-orbital centered on one of the bonds

s-orbital centered on one of the bonds

s-orbital centered on one of the bonds

SIESTA variables related with the wannierization

41 2009 = orbitals in unit cell and supercell. See end of file.

io	ia	is	spec	iao	n	l	m	z	p	sym	rc	isc			iuo
1	1	1	B	1	2	0	0	1	F	s	4.997	0	0	0	1
2	1	1	B	2	2	0	0	2	F	s	3.572	0	0	0	2
3	1	1	B	3	2	1	-1	1	F	py	5.996	0	0	0	3
4	1	1	B	4	2	1	0	1	F	pz	5.996	0	0	0	4
5	1	1	B	5	2	1	1	1	F	px	5.996	0	0	0	5
6	1	1	B	6	2	1	-1	2	F	py	4.287	0	0	0	6
7	1	1	B	7	2	1	0	2	F	pz	4.287	0	0	0	7
8	1	1	B	8	2	1	1	2	F	px	4.287	0	0	0	8
9	1	1	B	9	3	2	-2	1	T	Pdxy	5.996	0	0	0	9
10	1	1	B	10	3	2	-1	1	T	Pdyz	5.996	0	0	0	10
11	1	1	B	11	3	2	0	1	T	Pdz2	5.996	0	0	0	11
12	1	1	B	12	3	2	1	1	T	Pdxz	5.996	0	0	0	12
13	1	1	B	13	3	2	2	1	T	Pdx2-y2	5.996	0	0	0	13
14	2	2	N	1	2	0	0	1	F	s	3.767	0	0	0	14
15	2	2	N	2	2	0	0	2	F	s	2.568	0	0	0	15
16	2	2	N	3	2	1	-1	1	F	py	4.511	0	0	0	16
17	2	2	N	4	2	1	0	1	F	pz	4.511	0	0	0	17
18	2	2	N	5	2	1	1	1	F	px	4.511	0	0	0	18
19	2	2	N	6	2	1	-1	2	F	py	3.060	0	0	0	19
20	2	2	N	7	2	1	0	2	F	pz	3.060	0	0	0	20
21	2	2	N	8	2	1	1	2	F	px	3.060	0	0	0	21
22	2	2	N	9	3	2	-2	1	T	Pdxy	4.511	0	0	0	22
23	2	2	N	10	3	2	-1	1	T	Pdyz	4.511	0	0	0	23
24	2	2	N	11	3	2	0	1	T	Pdz2	4.511	0	0	0	24
25	2	2	N	12	3	2	1	1	T	Pdxz	4.511	0	0	0	25
26	2	2	N	13	3	2	2	1	T	Pdx2-y2	4.511	0	0	0	26
27	3	3	Ghost-	1	1	0	0	1	F	s	4.927	0	0	0	27
28	3	3	Ghost-	2	1	0	0	2	F	s	3.397	0	0	0	28
29	3	3	Ghost-	3	2	1	-1	1	T	Ppy	4.927	0	0	0	29
30	3	3	Ghost-	4	2	1	0	1	T	Ppz	4.927	0	0	0	30
31	3	3	Ghost-	5	2	1	1	1	T	Ppx	4.927	0	0	0	31
32	4	3	Ghost-	1	1	0	0	1	F	s	4.927	0	0	0	32
33	4	3	Ghost-	2	1	0	0	2	F	s	3.397	0	0	0	33
34	4	3	Ghost-	3	2	1	-1	1	T	Ppy	4.927	0	0	0	34
35	4	3	Ghost-	4	2	1	0	1	T	Ppz	4.927	0	0	0	35
36	4	3	Ghost-	5	2	1	1	1	T	Ppx	4.927	0	0	0	36
37	5	3	Ghost-	1	1	0	0	1	F	s	4.927	0	0	0	37
38	5	3	Ghost-	2	1	0	0	2	F	s	3.397	0	0	0	38
39	5	3	Ghost-	3	2	1	-1	1	T	Ppy	4.927	0	0	0	39
40	5	3	Ghost-	4	2	1	0	1	T	Ppz	4.927	0	0	0	40
41	5	3	Ghost-	5	2	1	1	1	T	Ppx	4.927	0	0	0	41

A good initial guess to project the bands of the higher band of the VB is the pz-orbital centered on the N atom

Take a look to the SystemLabel.ORB_INDX file

p_z-orbitals of the N atom

SIESTA variables related with the wannierization

```
%block Wannier.manifold.first
 bands    1     4                  # Indices of the initial and final
                                   # band of the manifold
  trial-orbitals  [27, 32, 37, 20] # Indices of the orbitals that will
                                   # be used as localized trial orbitals
                                   # See h-BN.ORB_INDX file
                                   # 27 : 1s-orbital Ghost-H atom
                                   # 32 : 1s-orbital Ghost-H atom
                                   # 37 : 1s-orbital Ghost-H atom
                                   # 20 : 2pz-orbital N atom
  spreading.nitt     0             # Number of iterations for the minimization of \Omega
  fermi_surface_plot false         # Plot the Fermi surface (False -> NO)
  wannier_plot   3                 # Plot the Wannier function
  write_hr true                    # Write the Hamiltonian in the WF basis
  write_tb true                    # Write the Hamiltonian in the WF basis
%endblock
```

Number of iterations for the minimization of the localization functional

If zero, then the procedure is the same as a Löwdin orthonormalization

The resulting Wannier functions will keep the symmetry of the projection function, but it will not be maximally localized

SIESTA variables related with the wannierization

```
%block Wannier.manifold.first
 bands    1     4                  # Indices of the initial and final
                                   # band of the manifold
  trial-orbitals  [27, 32, 37, 20] # Indices of the orbitals that will
                                   # be used as localized trial orbitals
                                   # See h-BN.ORB_INDX file
                                   # 27 : 1s-orbital Ghost-H atom
                                   # 32 : 1s-orbital Ghost-H atom
                                   # 37 : 1s-orbital Ghost-H atom
                                   # 20 : 2pz-orbital N atom
  spreading.nitt     0             # Number of iterations for the minimization of \Omega
  fermi_surface_plot false         # Plot the Fermi surface (False -> NO)
  wannier_plot   3                 # Plot the Wannier function
  write_hr true                    # Write the Hamiltonian in the WF basis
  write_tb true                    # Write the Hamiltonian in the WF basis
%endblock
```

Flag to determine whether the Fermi Surface is computed or not

SIESTA variables related with the wannierization

```
%block Wannier.manifold.first
 bands    1     4                    # Indices of the initial and final
                                     # band of the manifold
  trial-orbitals  [27, 32, 37, 20]   # Indices of the orbitals that will
                                     # be used as localized trial orbitals
                                     # See h-BN.ORB_INDX file
                                     # 27 : 1s-orbital Ghost-H atom
                                     # 32 : 1s-orbital Ghost-H atom
                                     # 37 : 1s-orbital Ghost-H atom
                                     # 20 : 2pz-orbital N atom
  spreading.nitt     0               # Number of iterations for the minimization of \Omega
  fermi_surface_plot false           # Plot the Fermi surface (False -> NO)
  wannier_plot   3                   # Plot the Wannier function
  write_hr true                      # Write the Hamiltonian in the WF basis
  write_tb true                      # Write the Hamiltonian in the WF basis
%endblock
```

Instruction to plot the Wannier functions

The integer refers to the size of the supercell for plotting the Wannier functions

SIESTA variables related with the wannierization

```
%block Wannier.manifold.first
 bands    1     4                    # Indices of the initial and final
                                     # band of the manifold
  trial-orbitals  [27, 32, 37, 20]   # Indices of the orbitals that will
                                     # be used as localized trial orbitals
                                     # See h-BN.ORB_INDX file
                                     # 27 : 1s-orbital Ghost-H atom
                                     # 32 : 1s-orbital Ghost-H atom
                                     # 37 : 1s-orbital Ghost-H atom
                                     # 20 : 2pz-orbital N atom
  spreading.nitt     0               # Number of iterations for the minimization of \Omega
  fermi_surface_plot false           # Plot the Fermi surface (False -> NO)
  wannier_plot   3                   # Plot the Wannier function
  write_hr true                      # Write the Hamiltonian in the WF basis
  write_tb true                      # Write the Hamiltonian in the WF basis
%endblock
```

Flag to determine whether the Hamiltonian in real space in a basis of Wannier functions is written

SystemLabel.manifold.X_hr.dat

X is the nickname of the manifold

SIESTA variables related with the wannierization

```
%block Wannier.manifold.first
 bands    1     4                    # Indices of the initial and final
                                     # band of the manifold
  trial-orbitals  [27, 32, 37, 20]   # Indices of the orbitals that will
                                     # be used as localized trial orbitals
                                     # See h-BN.ORB_INDX file
                                     # 27 : 1s-orbital Ghost-H atom
                                     # 32 : 1s-orbital Ghost-H atom
                                     # 37 : 1s-orbital Ghost-H atom
                                     # 20 : 2pz-orbital N atom
  spreading.nitt     0               # Number of iterations for the minimization of \Omega
  fermi_surface_plot false           # Plot the Fermi surface (False -> NO)
  wannier_plot   3                   # Plot the Wannier function
  write_hr true                      # Write the Hamiltonian in the WF basis
  write_tb true                      # Write the Hamiltonian in the WF basis
%endblock
```

Flag to determine whether the lattice vectors, Hamiltonian in real space and position operator in a basis of Wannier functions are written

SystemLabel.manifold.X_tb.dat

X is the nickname of the manifold

SIESTA variables related with the wannierization

```
Wannier.k [10 10 1]
```

Number of k-points used in the Wannierization

Succesful output of SIESTA

```
switch_local_projection: Populating the relevant matrices for
switch_local_projection: calling WANNIER90 directly from SIESTA
switch_local_projection: band manifold = first

compute_pw_matrix: Computing the matrix elements of a plane wave

mmn: Overlap matrices between periodic part of wavefunctions
mmn: written in h-BN.manifold.first.mmn file
Registered Wannier projectors for manifold 1:
    66       wann_orb  0  0  4.9274
    67       wann_orb  0  0  4.9274
    68       wann_orb  0  0  4.9274
    69       wann_orb  1  0  3.0605

amn: Overlap matrices between trial projection functions and wavefunctions
amn: written in h-BN.manifold.first.amn file

eig: Eigenvalues of the Hamiltonian
eig: written in h-BN.manifold.first.eigW file

compute_matrices: All the information dumped in the corresponding files
compute_matrices: End of the interface between Siesta and Wannier90
... Calling wannier90 for this manifold
... See file h-BN.manifold.first.wout for information
```

Succesful output of SIESTA

```
*------------------------------ WANNIERISE ------------------------------*
+-------------------------------------------------------------------+<-- CONV
| Iter  Delta Spread     RMS Gradient      Spread (Ang^2)      Time  |<-- CONV
+-------------------------------------------------------------------+<-- CONV

-----------------------------------------------------------------------
Initial State
 WF centre and spread    1  (  2.352380, -0.000000,  0.000000 )     0.58944034
 WF centre and spread    2  (  0.992353, -0.785204,  0.000000 )     0.58942901
 WF centre and spread    3  (  0.992353,  0.785204,  0.000000 )     0.58942901
 WF centre and spread    4  (  2.891390, -0.000000, -0.000000 )     1.36157867
 Sum of centres and spreads (  7.228475, -0.000000,  0.000000 )     3.12987704

     0     0.313E+01     0.0000000000        3.1298770370       0.00  <-- CONV
       O_D=      0.0611328 O_OD=      0.5126071 O_TOT=      3.1298770 <-- SPRD
-----------------------------------------------------------------------
Final State
 WF centre and spread    1  (  2.352380, -0.000000,  0.000000 )     0.58944034
 WF centre and spread    2  (  0.992353, -0.785204,  0.000000 )     0.58942901
 WF centre and spread    3  (  0.992353,  0.785204,  0.000000 )     0.58942901
 WF centre and spread    4  (  2.891390, -0.000000, -0.000000 )     1.36157867
 Sum of centres and spreads (  7.228475, -0.000000,  0.000000 )     3.12987704

       Spreads (Ang^2)       Omega I      =     2.556137111
      ================       Omega D      =     0.061132794
                             Omega OD     =     0.512607133
   Final Spread (Ang^2)      Omega Total  =     3.129877037
-----------------------------------------------------------------------
Time for wannierise            0.001 (sec)

done
```

The output is exactly the same as the WANNIER90 code h-BN.manifold.first.wout

3 WF centered on the B-N bonds
The spread of the Wannier functions (in Å) is three fold degenerated

Succesful output of SIESTA

```
*------------------------------ WANNIERISE ------------------------------*
+-------------------------------------------------------------------+<-- CONV
| Iter   Delta Spread      RMS Gradient      Spread (Ang^2)      Time  |<-- CONV
+-------------------------------------------------------------------+<-- CONV

-----------------------------------------------------------------------
Initial State
 WF centre and spread    1  (  2.352380, -0.000000,  0.000000 )     0.58944034
 WF centre and spread    2  (  0.992353, -0.785204,  0.000000 )     0.58942901
 WF centre and spread    3  (  0.992353,  0.785204,  0.000000 )     0.58942901
 WF centre and spread    4  (  2.891390, -0.000000, -0.000000 )     1.36157867
 Sum of centres and spreads (  7.228475, -0.000000,  0.000000 )     3.12987704

     0     0.313E+01     0.0000000000        3.1298770370       0.00  <-- CONV
       O_D=      0.0611328 O_OD=      0.5126071 O_TOT=      3.1298770 <-- SPRD
-----------------------------------------------------------------------
Final State
 WF centre and spread    1  (  2.352380, -0.000000,  0.000000 )     0.58944034
 WF centre and spread    2  (  0.992353, -0.785204,  0.000000 )     0.58942901
 WF centre and spread    3  (  0.992353,  0.785204,  0.000000 )     0.58942901
 WF centre and spread    4  (  2.891390, -0.000000, -0.000000 )     1.36157867
 Sum of centres and spreads (  7.228475, -0.000000,  0.000000 )     3.12987704

        Spreads (Ang^2)       Omega I      =     2.556137111
       ================       Omega D      =     0.061132794
                              Omega OD     =     0.512607133
   Final Spread (Ang^2)       Omega Total  =     3.129877037
-----------------------------------------------------------------------
Time for wannierise            0.001 (sec)

done
```

The output is exactly the same as the WANNIER90 code h-BN.manifold.first.wout

1 WF centered on the N atom

How to plot the Wannier functions

First of all, SIESTA has to write the periodic part of the Bloch functions in a 3D grid. The number of points in the grid along the three lattice vectors are given by

seedname.fdf file
(input of SIESTA)

```
Wannier.Manifolds.Unk .true.

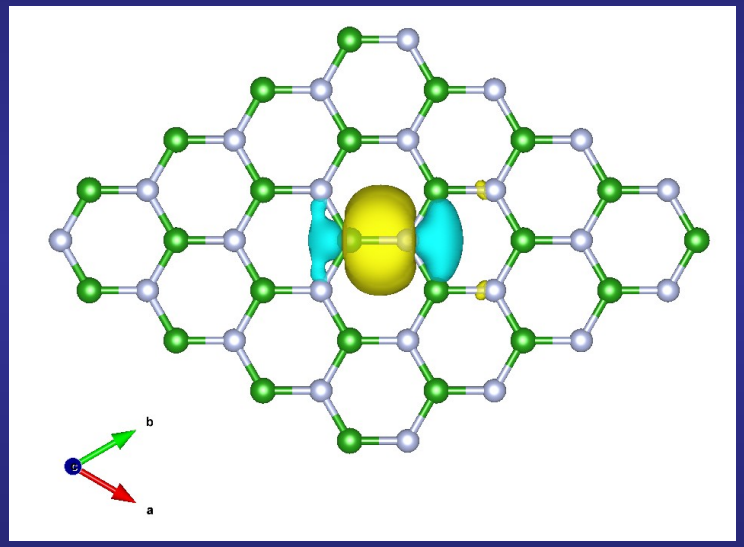
Siesta2Wannier90.UnkGrid1 30
Siesta2Wannier90.UnkGrid2 30
Siesta2Wannier90.UnkGrid3 30
```

This produces many files with the name UNKXXXXX.Y where

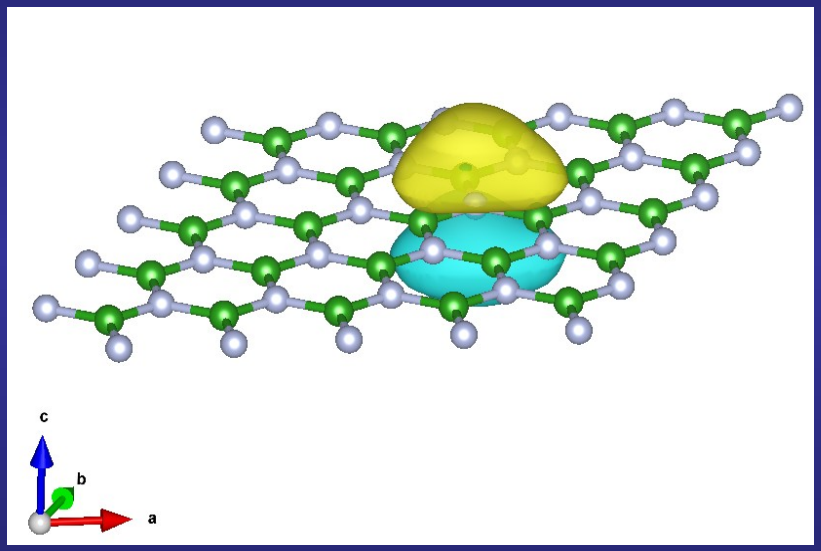
- **XXXXX is the number of the k-point, from 1 to the number of points included in seedname.win file**
- **Y refers to the spin compoment (1 or 2)**

Wannier functions

sp^2-orbital



π-orbital



How to plot the Wannier functions

First of all, SIESTA has to write the periodic part of the Bloch functions in a 3D grid. The number of points in the grid along the three lattice vectors are given by

seedname.fdf file
(input of SIESTA)

```
Wannier.Manifolds.Unk .true.

Siesta2Wannier90.UnkGrid1 30
Siesta2Wannier90.UnkGrid2 30
Siesta2Wannier90.UnkGrid3 30
```

This produces many files with the name UNKXXXXX.Y where

- **XXXXX is the number of the k-point, from 1 to the number of points included in seedname.win file**
- **Y refers to the spin compoment (1 or 2)**

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